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# SEMIRELATIVISTIC TREATMENT OF BOUND STATES

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## Abstract

This talk reviews several aspects of the “semirelativistic” description of bound states by the spinless Salpeter equation (which represents the simplest equation of motion incorporating relativistic effects) and, in particular, presents or recalls some very simple and elementary methods which allow to derive rigorous statements on the corresponding solutions, that is, on energy levels as well as wave functions.

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# 1 SPINLESS SALPETER EQUATION

The conceptually simplest bound-state wave equation incorporating to some extent relativistic effects is the “spinless Salpeter equation.” The origin of this equation of motion is by no means some mystery. Rather, this spinless Salpeter equation has to be regarded as a well-defined standard approximation to the Bethe–Salpeter formalism.

## 1.1 Bethe–Salpeter (BS) Formalism

The appropriate framework for the description of bound states within some relativistic quantum field theory is the Bethe–Salpeter formalism. Consider the bound state  $|M\rangle$  (with momentum  $K$  and energy  $E$ ) of, say, (spin- $\frac{1}{2}$ ) fermion and antifermion (with masses  $M_1, M_2$  and momenta  $P_1, P_2$ , respectively). Within the BS formalism this bound state is represented by its *Bethe–Salpeter amplitude*  $\Psi$  which, in momentum space, is defined as Fourier transform of the time-ordered product of the field operators of the two bound-state constituents between the vacuum  $|0\rangle$  and the bound state, after factorizing off the center-of-momentum motion:

$$\Psi(P) = \exp(i K X_{\text{CM}}) \int d^4 X \exp(i P X) \langle 0 | T(\psi_1(X_1) \bar{\psi}_2(X_2)) | M(K) \rangle ,$$

with the usual kinematical notions of total momentum  $K = P_1 + P_2$ , relative momentum  $P$ , center-of-momentum coordinate  $X_{\text{CM}}$ , and relative coordinate  $X \equiv X_1 - X_2$  of the bound-state constituents.

The BS amplitude  $\Psi$  satisfies the *Bethe–Salpeter equation* [1]

$$S_1^{-1}(P_1) \Psi(P) S_2^{-1}(-P_2) = \frac{i}{(2\pi)^4} \int d^4 Q \mathcal{K}(P, Q) \Psi(Q) ,$$

which involves two dynamical ingredients, namely,

- on the one hand, the full fermion propagator of particle  $i$  ( $i = 1, 2$ ), denoted by  $S(P, M)$  for any particle of momentum  $P$  and mass  $M$ , which, however, is usually approximated by its free form

$$S_0^{-1}(P, M) = -i(\gamma_\mu P^\mu - M) ,$$

with  $M$  interpreted as some effective (“constituent”) mass and the propagator  $S_0$  understood as an effective one, and,

- on the other hand, the *BS interaction kernel*  $\mathcal{K}(P, Q)$ , which is defined (only perturbatively!) as sum of all two-particle (“BS-”) irreducible Feynman diagrams for two-particle into two-particle scattering (exhibiting, consequently, a certain amount of gauge dependence), and which is given, for instance, in lowest order quantum electrodynamics from one-photon exchange (in Feynman gauge) by

$$\mathcal{K}(P, Q) = \frac{e^2}{(P - Q)^2} \gamma^\mu \otimes \gamma_\mu .$$

By construction, the BS equation is formally exact. Its actual application, however, faces several, rather well-known **problems**:<sup>1</sup>

- There is no means to compute the BS kernel beyond the very tight limits of perturbation theory.
- Even with the BS kernel at one’s disposal, it is, in general, not possible to find the exact solutions of the BS equation (except for rather few special cases, like the famous Wick–Cutkosky model describing the interaction of two scalar particles by exchange of some massless scalar particle).
- In non-Abelian gauge theories like, e.g., quantum chromodynamics, since the Dyson–Schwinger equations connect the propagators and the interaction kernel, the simultaneous assumption of free propagators and a confining BS kernel is obviously inconsistent.

The most straightforward way out is the **reduction** of the Bethe–Salpeter equation by a series of approximations:

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<sup>1</sup> The appearance of states with negative or vanishing norm among the obtained solutions as well as questions of interpretation, for instance, cause additional troubles when dealing with the BS equation.

1. Eliminate any dependence on timelike variables. This (innocent) enterprise involves two steps:

- Adhere to the *static approximation* to the BS kernel (which has to be justified *a posteriori*), that is, assume that the BS kernel depends only on the relative three-momenta  $\mathbf{Q}$  and  $\mathbf{P}$  of initial and final state, respectively:

$$\mathcal{K}(P, Q) = \mathcal{K}(\mathbf{P}, \mathbf{Q}) .$$

(This amounts to ignoring all retardation effects by assuming instantaneous interactions.)

- Define the *equal-time wave function*  $\Phi$ , sometimes also called the “Salpeter amplitude,” (in momentum space) by integrating the BS amplitude  $\Psi(P)$  over the zero component of the four-momentum  $P$ :

$$\Phi(\mathbf{P}) \equiv \int dP_0 \Psi(\mathbf{P}, P_0) .$$

This leads to the *Salpeter equation* [2]

$$\Phi(\mathbf{P}) = \int \frac{d^3Q}{(2\pi)^3} \left[ \frac{\Lambda_1^+ \gamma_0 \mathcal{K}(\mathbf{P}, \mathbf{Q}) \Phi(\mathbf{Q}) \gamma_0 (\Lambda_2^+)^c}{E - \sqrt{\mathbf{P}_1^2 + M_1^2} - \sqrt{\mathbf{P}_2^2 + M_2^2}} - \frac{\Lambda_1^- \gamma_0 \mathcal{K}(\mathbf{P}, \mathbf{Q}) \Phi(\mathbf{Q}) \gamma_0 (\Lambda_2^-)^c}{E + \sqrt{\mathbf{P}_1^2 + M_1^2} + \sqrt{\mathbf{P}_2^2 + M_2^2}} \right] ,$$

with the energy projection operators for positive or negative energy of particle  $i$  ( $i = 1, 2$ ) given, as usual, by

$$\Lambda_i^\pm \equiv \frac{\sqrt{\mathbf{P}_i^2 + M_i^2} \pm \gamma_0 (\boldsymbol{\gamma} \cdot \mathbf{P}_i + M_i)}{2 \sqrt{\mathbf{P}_i^2 + M_i^2}}$$

and

$$(\Lambda_i^\pm)^c \equiv (C^{-1} \Lambda_i^\pm C)^T = \Lambda_i^\mp ,$$

where  $C$  is the charge conjugation matrix. The Salpeter equation is the equation of motion for the equal-time wave function  $\Phi(\mathbf{P})$ , with full relativistic kinematics but in static approximation for the interaction kernel  $\mathcal{K}$ .

2. Neglect the second term on the right-hand side of the Salpeter equation on the basis of the—at least for “heavy” bound-state constituents reasonable—assumption that the denominator of the first term is much smaller than the denominator of the second term:

$$E - \sqrt{\mathbf{P}_1^2 + M_1^2} - \sqrt{\mathbf{P}_2^2 + M_2^2} \ll E + \sqrt{\mathbf{P}_1^2 + M_1^2} + \sqrt{\mathbf{P}_2^2 + M_2^2} .$$

This leads to the *reduced Salpeter equation*

$$\boxed{\left( E - \sqrt{\mathbf{P}_1^2 + M_1^2} - \sqrt{\mathbf{P}_2^2 + M_2^2} \right) \Phi(\mathbf{P}) = \int \frac{d^3Q}{(2\pi)^3} \Lambda_1^+ \gamma_0 \mathcal{K}(\mathbf{P}, \mathbf{Q}) \Phi(\mathbf{Q}) \gamma_0 (\Lambda_2^+)^c} .$$

3. Neglect any reference to the spin degrees of freedom of the involved bound-state constituents.
4. Assume that the BS kernel  $\mathcal{K}(\mathbf{P}, \mathbf{Q})$  depends only on the difference of the relative momenta  $\mathbf{P}$  and  $\mathbf{Q}$ , which means that the BS kernel is of convolution type (as is, in fact, frequently the case):

$$\mathcal{K}(\mathbf{P}, \mathbf{Q}) = \mathcal{K}(\mathbf{P} - \mathbf{Q}) .$$

5. Restrict the whole formalism exclusively to positive-energy solutions, which will be denoted by  $\psi$ .

After applying all these simplifying assumptions and approximations to the BS equation, one finally ends up with the *spinless Salpeter equation*

$$\boxed{\left[ \sqrt{\mathbf{P}_1^2 + M_1^2} + \sqrt{\mathbf{P}_2^2 + M_2^2} + V(\mathbf{X}) \right] \psi = E \psi} ,$$

involving an interaction potential,  $V(\mathbf{X})$ , arising as the Fourier transform of the BS kernel  $\mathcal{K}(\mathbf{P} - \mathbf{Q})$ . In particular, in the center-of-momentum frame of the two bound-state constituents (i.e., for  $\mathbf{K} = \mathbf{0}$ ), this equation reads

$$H|\psi\rangle = E|\psi\rangle ,$$

with the Hamiltonian

$$H = \sqrt{\mathbf{P}^2 + M_1^2} + \sqrt{\mathbf{P}^2 + M_2^2} + V(\mathbf{X}) .$$

## 1.2 Equal-Mass Case

For the special case of equal masses of the two involved bound-state constituents, i.e., when assuming

$$M_1 = M_2 = M ,$$

it is possible to recast the two-particle spinless Salpeter equation into the equivalent one-particle form. In order to see this, consider the semirelativistic Hamiltonian  $H$  for the two-particle spinless Salpeter equation with an interaction described by a central potential  $V(|\mathbf{X}|)$  of, for instance, power-law form:

$$H = 2 \sqrt{\mathbf{P}^2 + M^2} + \sum_{n \in \mathbb{Z}} k_n R^n , \quad R \equiv |\mathbf{X}| .$$

One may always perform a scale transformation of the phase-space variables  $\mathbf{X}, \mathbf{P}$  by some arbitrary scale factor  $\lambda$ ,

$$\mathbf{p} = \lambda \mathbf{P} , \quad \mathbf{x} = \frac{\mathbf{X}}{\lambda} ,$$

since any transformation of this kind (necessarily) preserves the fundamental commutation relations:

$$[\mathbf{x}, \mathbf{p}] = [\mathbf{X}, \mathbf{P}] .$$

Now,

- fix the scale parameter  $\lambda$  to the value  $\lambda = 2$ , which implies for the semirelativistic Hamiltonian

$$\begin{aligned} H &= \sqrt{4 \mathbf{P}^2 + 4 M^2} + \sum_{n \in \mathbb{Z}} k_n R^n \\ &= \sqrt{\mathbf{p}^2 + 4 M^2} + \sum_{n \in \mathbb{Z}} k_n 2^n r^n , \end{aligned}$$

- identify the mass and coupling-strength parameters for one- and two-particle form according to

$$\begin{aligned} m &= 2 M , \\ a_n &= 2^n k_n , \quad n \in \mathbb{Z} , \end{aligned}$$

and arrive—presumably without great surprise—at the equivalent one-particle Hamiltonian

$$H = \sqrt{\mathbf{p}^2 + m^2} + \sum_{n \in \mathbb{Z}} a_n r^n , \quad r \equiv |\mathbf{x}| .$$

## 1.3 (One-Particle) Spinless Salpeter Equation

In view of the above observation, it is sufficient to confine the present discussion to the consideration of some self-adjoint Hamiltonian  $H$  of the form

$$H = T + V , \tag{1}$$

where  $T$  denotes the “square-root” operator of the relativistic expression for the free (kinetic) energy of some particle of mass  $m$  and momentum  $\mathbf{p}$ ,

$$T = T(\mathbf{p}) \equiv \sqrt{\mathbf{p}^2 + m^2} ,$$

and  $V = V(\mathbf{x})$  represents some arbitrary coordinate-dependent, static interaction-potential operator. The **spinless Salpeter equation** is nothing else but the eigenvalue equation for the Hamiltonian  $H$ ,

$$H|\chi_k\rangle = E_k|\chi_k\rangle , \quad k = 0, 1, 2, \dots ,$$

for the (complete set of) Hilbert-space eigenvectors  $|\chi_k\rangle$  of  $H$  corresponding to the energy eigenvalues

$$E_k \equiv \frac{\langle \chi_k | H | \chi_k \rangle}{\langle \chi_k | \chi_k \rangle} .$$

As such, it represents the simplest relativistic generalization of the Schrödinger equation of standard nonrelativistic quantum theory. **N.B.** The semirelativistic Hamiltonian  $H$  is a *nonlocal* operator, i.e.,

- either the relativistic kinetic-energy operator  $T$  *in configuration space*
- or, in general, the interaction-potential operator  $V$  *in momentum space*

is nonlocal. Because of this nonlocality it is somewhat difficult to obtain rigorous *analytic* statements on the solutions of this equation of motion.

## 2 RELATIVISTIC COULOMB PROBLEM

Of particular importance in many realms of physics is the (spherically symmetric) Coulomb potential, with interaction strength parametrized by some dimensionless coupling (“fine structure”) constant  $\alpha$ :

$$V(\mathbf{x}) = V_C(r) = -\frac{\alpha}{r}, \quad r \equiv |\mathbf{x}|, \quad \alpha > 0. \quad (2)$$

### 2.1 Spinless Relativistic Coulomb Problem

Since we will use the Coulomb potential in order to illustrate the general statements derived below, let us briefly summarize, in roughly chronological order, the most important knowledge gained until now:

- By examination of the spectral properties of the semirelativistic Hamiltonian  $H$  with a Coulomb interaction potential  $V_C(r)$ , one is able to prove [3] for this operator  $H$

- its *essential self-adjointness* (which means that the closure of  $H$  is self-adjoint) for  $\alpha \leq \frac{1}{2}$ ;
- the existence of its *Friedrichs extension* up to a critical value  $\alpha_c$  of the coupling constant  $\alpha$ :

$$\alpha_c = \frac{2}{\pi};$$

- a strict *lower bound* on the ground-state energy  $E_0$  (that is, on the operator  $H$ ), given by

$$E_0 \geq m \sqrt{1 - \left(\frac{\pi \alpha}{2}\right)^2} \quad \text{for } \alpha < \frac{2}{\pi}.$$

Loosely speaking, the Coulombic Hamiltonian  $H$  may be regarded as reasonable operator up to the critical coupling constant  $\alpha_c$ .

- For part of the allowed range of the coupling constant  $\alpha$ , an improved lower bound can be found [4]:

$$E_0 \geq m \sqrt{\frac{1 + \sqrt{1 - 4\alpha^2}}{2}} \quad \text{for } \alpha < \frac{1}{2}.$$

- The analytic solution for the corresponding wave function  $\psi$  has been constructed [5]; inspecting its behaviour near the origin, one observes for, e.g., vanishing orbital angular momentum ( $\ell = 0$ ) that the configuration-space wave function  $\psi(\mathbf{x})$  diverges for small values of  $r \equiv |\mathbf{x}|$  exactly like

$$\lim_{r \rightarrow 0} \psi(\mathbf{x}) \propto r^{-\nu} \quad \text{with} \quad \nu = \frac{2\alpha}{\pi} \left(1 + \frac{2\alpha}{\pi} + \dots\right).$$

- Given the relative uselessness of Temple’s inequality, lower bounds on the spectrum of  $H$  may be found (in a numerical manner) with the help of the **generalized “local-energy” theorem** [6]:

- Assume
  1. that the Fourier transform  $\tilde{V}(\mathbf{p})$  of the interaction potential  $V(\mathbf{x})$  is strictly negative, except at infinity, as is (certainly) the case for the (attractive) Coulomb potential (2),
  2. that the spectrum of the operator  $H$  is discrete, and
  3. that the ground state of the Hamiltonian  $H$  exists.
- Define the “local energy”

$$\mathcal{E}(\mathbf{p}) \equiv T(\mathbf{p}) + \frac{\int d^3q \tilde{V}(\mathbf{p} - \mathbf{q}) \phi(\mathbf{q})}{\phi(\mathbf{p})},$$

where  $\phi(\mathbf{p})$  denotes some suitably chosen, positive trial function,

$$\phi(\mathbf{p}) > 0.$$

Then the lowest-lying eigenvalue  $E_0$  of the Hamiltonian  $H$  is bounded from below and above by<sup>2</sup>

$$\inf_{\mathbf{p}} \mathcal{E}(\mathbf{p}) \leq E_0 < \sup_{\mathbf{p}} \mathcal{E}(\mathbf{p}).$$

<sup>2</sup> The lower bound even holds if the assumption on the discreteness of the spectrum is not fulfilled.

Table 1: Numerically (!) obtained [6] lower and upper bounds on the ground-state energy  $E_0(\alpha)$ 

$\alpha$	$\frac{E_0}{m}$	
	Lower Bound	Upper Bound
0.0155522	0.9998785	0.9998791
0.1425460	0.989458	0.989613
0.2599358	0.96309	0.96364
0.3566678	0.92578	0.92673
0.4359255	0.88013	0.88139
0.5	0.82758	0.82910
0.5505528	0.76908	0.77075
0.5887832	0.7050	0.7069
0.6155367	0.6359	0.6379
0.6313752	0.5616	0.5637
0.6366198	0.4825	0.4843

With the help of this local-energy theorem, the ground-state energy, considered as a function  $E_0(\alpha)$  of the coupling strength  $\alpha$ , has been restricted to some remarkably narrow band (Table 1). In particular, at the critical coupling constant  $\alpha_c$  one finds

$$0.4825 \leq \frac{E_0(\alpha = \alpha_c)}{m} \leq 0.4842910 \quad \text{for } \alpha = \alpha_c .$$

From this one learns that the ground-state energy  $E_0$  at the critical coupling constant  $\alpha_c$  is definitely nonvanishing (which is evidently *not* clear from the lower bounds quoted above).

## 2.2 Power Series Expansions

The systematic series expansions of the energy eigenvalues  $E(n_r, \ell)$  in powers of the coupling constant  $\alpha$  (up to and including the order  $O(\alpha^7)$ ) for states with radial quantum number  $n_r$  and orbital angular momentum  $\ell$  have been worked out in different ways [7, 8]. The **disadvantage** of these power-series expansions is that they are only significant for a region of rather small values of the coupling constant  $\alpha$ . These expansions read, for instance,

- for  $n_r = 0, \ell = 0$  (i.e., for the ground state):

$$\begin{aligned} \frac{E(n_r = 0, \ell = 0)}{m} &= 1 - \frac{\alpha^2}{2} - \frac{5\alpha^4}{8} + \frac{8\alpha^5}{3\pi} + \alpha^6 \ln \alpha \\ &+ \left( \frac{7}{\pi^2} \zeta(3) - \frac{2}{\pi^2} - \frac{33}{16} \right) \alpha^6 + O(\alpha^7) , \end{aligned}$$

where  $\zeta(z)$  is the Riemann zeta function

$$\zeta(z) = \sum_{k=1}^{\infty} k^{-z} , \quad \Re z > 1 ,$$

which coincides up to order  $O(\alpha^4)$  with the improved lower bound on the ground-state energy;

- for  $n_r = 1, \ell = 0$ :

$$\begin{aligned} \frac{E(n_r = 1, \ell = 0)}{m} &= 1 - \frac{\alpha^2}{8} - \frac{13\alpha^4}{128} + \frac{\alpha^5}{3\pi} + \frac{\alpha^6 \ln \alpha}{8} \\ &+ \left( \frac{7}{8\pi^2} \zeta(3) - \frac{1}{4\pi^2} - \frac{197}{1024} - \frac{\ln 2}{8} \right) \alpha^6 + O(\alpha^7) ; \end{aligned}$$

- for  $n_r = 0, \ell = 1$ , where, remarkably, there are no contributions of the order  $O(\alpha^5)$  or  $O(\alpha^6 \ln \alpha)$ :

$$\frac{E(n_r = 0, \ell = 1)}{m} = 1 - \frac{\alpha^2}{8} - \frac{7\alpha^4}{384} + \frac{727\alpha^6}{82944} + O(\alpha^7) .$$

In any case, even for the Coulomb potential (2) the eigenvalues of the semirelativistic Hamiltonian (1) are not known exactly!

### 3 EXACT ANALYTIC UPPER BOUNDS ON ENERGY LEVELS

In view of the (admittedly rather unsatisfactory) state-of-the-art mentioned above, let us try to find, at least, exact upper bounds on the eigenvalues of the Hamiltonian (1) by entirely analytic methods. Clearly, the derivation of upper bounds on the eigenvalues of some operator only makes sense if this operator is bounded from below. Accordingly, let us assume that the (otherwise arbitrary) interaction potential  $V$  is such that the Hamiltonian  $H$  is bounded from below. For the **Coulomb potential** (2), the required semi-boundedness of the spectrum of the Hamiltonian  $H$  has been rigorously proven [3].

#### 3.1 Minimum–Maximum Principle

Beyond doubt, the theoretical foundation of (as well as the primary tool for) the derivation of rigorous upper bounds on the eigenvalues of some self-adjoint operator is the well-known “min–max principle.” There are several equivalent formulations of this theorem. For practical purposes, the most convenient one is the following:

- Let  $H$  be a self-adjoint operator bounded from below.
- Let  $E_k$ ,  $k = 0, 1, 2, \dots$ , denote the eigenvalues of  $H$ ,

$$H|\chi_k\rangle = E_k|\chi_k\rangle, \quad k = 0, 1, 2, \dots,$$

ordered according to

$$E_0 \leq E_1 \leq E_2 \leq \dots$$

- Let  $D_d$  be some  $d$ -dimensional subspace of the domain of  $H$ .

Then the  $k$ th eigenvalue  $E_k$  (counting multiplicity) of  $H$  satisfies the inequality

$$E_k \leq \sup_{|\psi\rangle \in D_{k+1}} \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad \text{for } k = 0, 1, 2, \dots$$

#### 3.2 Operator Inequalities

Needless to say, our goal must be to replace the problematic kinetic-energy square-root operator in the semirelativistic Hamiltonian  $H$  by some more tractable operator. One (obvious) way to achieve this is to use the min–max principle in order to compare eigenvalues of operators:

- Assume the validity of a generic operator inequality of the form

$$H \leq \mathcal{O}.$$

Then

$$\begin{aligned} E_k &\equiv \frac{\langle \chi_k | H | \chi_k \rangle}{\langle \chi_k | \chi_k \rangle} \\ &\leq \sup_{|\psi\rangle \in D_{k+1}} \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad (\text{by the min–max principle}) \\ &\leq \sup_{|\psi\rangle \in D_{k+1}} \frac{\langle \psi | \mathcal{O} | \psi \rangle}{\langle \psi | \psi \rangle} \quad (\text{by the operator inequality}). \end{aligned}$$

- Assume that the  $(k+1)$ -dimensional subspace  $D_{k+1}$  in these inequalities is spanned by the first  $k+1$  eigenvectors of the operator  $\mathcal{O}$ , that is, by precisely those eigenvectors of  $\mathcal{O}$  that correspond to the first  $k+1$  eigenvalues  $\hat{E}_0, \hat{E}_1, \dots, \hat{E}_k$  of  $\mathcal{O}$  if all eigenvalues of  $\mathcal{O}$  are ordered according to

$$\hat{E}_0 \leq \hat{E}_1 \leq \hat{E}_2 \leq \dots$$

Then

$$\sup_{|\psi\rangle \in D_{k+1}} \frac{\langle \psi | \mathcal{O} | \psi \rangle}{\langle \psi | \psi \rangle} = \hat{E}_k.$$

Consequently, every eigenvalue  $E_k$  of  $H$  is bounded from above by a corresponding eigenvalue  $\hat{E}_k$  of  $\mathcal{O}$ :

$$E_k \leq \hat{E}_k.$$

### 3.3 The “Schrödinger” Bound [9]

The simplest of all upper bounds on the eigenvalues of the semirelativistic Hamiltonian  $H$  of Eq. (1) is the one involving the corresponding “Schrödinger” Hamiltonian. It may be found by taking advantage of the positivity of the square of the (since  $T$  is self-adjoint, obviously self-adjoint) operator  $T - m$ :

$$\begin{aligned} 0 &\leq (T - m)^2 \\ &= T^2 + m^2 - 2mT \\ &\equiv \mathbf{p}^2 + 2m^2 - 2mT . \end{aligned}$$

Assuming  $m$  to be positive, this may be converted into an operator inequality for the kinetic energy  $T$ ,

$$T \leq m + \frac{\mathbf{p}^2}{2m} ,$$

which, in turn, entails an operator inequality for the (generic, since it involves an arbitrary interaction potential  $V$ ) Hamiltonian  $H$  in the spinless Salpeter equation [9]:

$$H \leq H_S ,$$

with the “Schrödinger” Hamiltonian

$$H_S = m + \frac{\mathbf{p}^2}{2m} + V .$$

For the **Coulomb potential** (2), the energy eigenvalues corresponding to the above Schrödinger Hamiltonian read

$$E_{S,n} = m \left( 1 - \frac{\alpha^2}{2n^2} \right) ,$$

where the total quantum number  $n$  is given in terms of both radial and orbital angular-momentum quantum numbers  $n_r$  and  $\ell$ , respectively, by

$$n = n_r + \ell + 1 , \quad n_r = 0, 1, 2, \dots , \quad \ell = 0, 1, 2, \dots .$$

### 3.4 A “Squared” Bound [9]

In order to improve the above bound, one might be tempted to consider the square of the Hamiltonian  $H$ :

$$Q \equiv H^2 = T^2 + V^2 + TV + VT .$$

The eigenvalue equation for this squared Hamiltonian  $Q$  will, of course, be solved by exactly the same set of eigenvectors  $|\chi_k\rangle$  as the one for the original Hamiltonian  $H$  with, however, the squares  $E_k^2$  of the corresponding energy eigenvalues  $E_k$  of  $H$  as the eigenvalues of  $Q$ :

$$Q|\chi_k\rangle = E_k^2|\chi_k\rangle , \quad k = 0, 1, 2, \dots .$$

The positivity of the square of the self-adjoint operator  $T - m - V$ ,

$$\begin{aligned} 0 &\leq (T - m - V)^2 \\ &= T^2 + m^2 + V^2 - 2mT + 2mV - TV - VT , \end{aligned}$$

and the (because of the positivity of the operator  $\mathbf{p}^2$  obviously valid) relation

$$0 \leq m \leq T$$

yield some operator inequality for the anticommutator  $TV + VT$  of kinetic energy  $T$  and interaction potential  $V$  showing up in the squared Hamiltonian  $Q$ :

$$\begin{aligned} TV + VT &\leq T^2 + m^2 + V^2 - 2mT + 2mV \\ &\equiv \mathbf{p}^2 + 2m^2 + V^2 - 2mT + 2mV \\ &\leq \mathbf{p}^2 + V^2 + 2mV . \end{aligned}$$



Insertion of this intermediate result implies an operator inequality for the squared Hamiltonian  $Q$  [9]:

$$Q \leq R ,$$

with the operator

$$R \equiv 2 \mathbf{p}^2 + m^2 + 2 V^2 + 2 m V .$$

According to the min–max principle, the squares of the energy eigenvalues  $E_k$  of the spinless Salpeter equation are therefore bounded from above by the corresponding eigenvalues  $\mathcal{E}_{R,k}$  of the operator  $R$ :

$$E_k^2 \leq \mathcal{E}_{R,k}$$

or

$$E_k \leq \sqrt{\mathcal{E}_{R,k}} .$$

Only for the **Coulomb potential** (2), the above operator  $R$  is of exactly the same structure as the “Schrödinger” Hamiltonian  $H_S$ , with, however, some “effective” orbital angular momentum quantum number  $L$  to be determined from the relation

$$L(L+1) = \ell(\ell+1) + \alpha^2 ,$$

with the result

$$L = \frac{\sqrt{1 + 4[\ell(\ell+1) + \alpha^2]} - 1}{2} , \quad \ell = 0, 1, 2, \dots .$$

The eigenvalues  $\mathcal{E}_R$  of the operator  $R$  may thus be found by replacing in the Coulomb eigenvalues  $E_{S,n}$  the angular momentum quantum number  $\ell$  by the effective angular momentum quantum number  $L$ :

$$\mathcal{E}_{R,N} = m^2 \left( 1 - \frac{\alpha^2}{2N^2} \right) ,$$

with the “effective” total quantum number  $N$  defined by

$$N = n_r + L + 1 , \quad n_r = 0, 1, 2, \dots .$$

Unfortunately, these “squared” bounds lie above and are thus worse than the “Schrödinger” bounds.

### 3.5 A Straightforward Generalization [9]

The “Schrödinger” bounds may be improved by generalizing a little bit the line of argument leading to their derivation. The positivity of the square of the (obviously self-adjoint) operator  $T - \mu$ , where  $\mu$  is an arbitrary real parameter (with the dimension of mass),

$$\begin{aligned} 0 &\leq (T - \mu)^2 \\ &= T^2 + \mu^2 - 2\mu T \\ &\equiv \mathbf{p}^2 + m^2 + \mu^2 - 2\mu T , \end{aligned}$$

implies a set of operator inequalities for the kinetic energy  $T$ :<sup>3</sup>

$$T \leq \frac{\mathbf{p}^2 + m^2 + \mu^2}{2\mu} \quad \text{for all } \mu > 0 .$$

This immediately translates into a set of operator inequalities for the semirelativistic Hamiltonian  $H$  [9]:

$$H \leq \hat{H}_S(\mu) \quad \text{for all } \mu > 0 ,$$

with the Schrödinger-like Hamiltonian

$$\hat{H}_S(\mu) = \frac{\mathbf{p}^2 + m^2 + \mu^2}{2\mu} + V .$$

Invoking again the min–max principle, any energy eigenvalue  $E_k$  of  $H$  is thus bounded from above by the corresponding eigenvalue  $\hat{E}_{S,k}(\mu)$  of the Schrödinger-like Hamiltonian  $\hat{H}_S(\mu)$  for given positive  $\mu$ ,

$$E_k \leq \hat{E}_{S,k}(\mu) \quad \text{for all } \mu > 0 ,$$

and—as a (trivial) consequence—also by the minimum of all these Schrödinger-like upper bounds [9]:

$$\boxed{E_k \leq \min_{\mu > 0} \hat{E}_{S,k}(\mu)} .$$

---

<sup>3</sup> See also Ref. [4].

For the **Coulomb potential** (2), it is trivial to write down the corresponding energy eigenvalues:

$$\hat{E}_{S,n}(\mu) = \frac{1}{2\mu} \left[ m^2 + \mu^2 \left( 1 - \frac{\alpha^2}{n^2} \right) \right],$$

with the total quantum number

$$n = n_r + \ell + 1.$$

Minimizing  $\hat{E}_{S,n}(\mu)$  with respect to the parameter  $\mu$  yields [9]

$$\boxed{\min_{\mu>0} \hat{E}_{S,n}(\mu) = m \sqrt{1 - \frac{\alpha^2}{n^2}}} \quad \text{for all } \alpha \leq \alpha_c. \quad (3)$$

These bounds

- hold for all values  $\alpha \leq \alpha_c$  of the Coulomb coupling constant  $\alpha$  and arbitrary levels of excitation, and
- improve definitely the Schrödinger bounds, for any value of the total (or “principal”) quantum number  $n$ :

$$\min_{\mu>0} \hat{E}_{S,n}(\mu) < E_{S,n} \quad \text{for } \alpha \neq 0.$$

(For  $\mu = m$  one necessarily recovers the Schrödinger case.) The **comparison** of the upper bounds of Eq. (3) with their numerically [6] or by a perturbative expansion [8] obtained counterparts shows that

1. for the ground state, i.e.,  $n_r = \ell = 0$ , hence  $n = 1$  (Table 2), the relative error of our analytical (operator) bound (in the considered range of the coupling constant  $\alpha$ ) is less than 4.5 %, and

Table 2: Numerical [6] vs. analytical upper bounds on the ground-state energy  $E_0$

$\alpha$	Upper Bound on $\frac{E_0}{m}$	
	Numerical	Analytical
0.0155522	0.9998791	0.9998791
0.1425460	0.989613	0.989788
0.2599358	0.96364	0.96563
0.3566678	0.92673	0.93423
0.4359255	0.88139	0.8998
0.5	0.82910	0.86603

2. for the level  $n_r = 0, \ell = 1$  and thus  $n = 2$  (Table 3) the relative error of our analytical (operator) bound (in the considered range of the coupling constant  $\alpha$ ) is less than 0.1 %.

Table 3: Perturbatively computed [8] energy eigenvalues vs. analytical upper bounds for  $n_r = 0, \ell = 1$

$\alpha$	$\frac{E(n_r = 0, \ell = 1)}{m}$	
	Perturbation Theory	Analytical Bound
0.0155522	0.999969765	0.999969766
0.1425460	0.997452	0.997457
0.2599358	0.99147	0.99152
0.3566678	0.9838	0.9840
0.4359255	0.975	0.976
0.5	0.967	0.9682

### 3.6 Rayleigh–Ritz Variational Technique

An **immediate consequence of the min–max principle** is the famous Rayleigh–Ritz technique:

- Restrict the operator  $H$  to the subspace  $D_d$  by orthogonal projection  $P$  onto  $D_d$ :

$$\hat{H} \equiv H \Big|_{D_d} := P H P .$$

- Let  $\hat{E}_k$ ,  $k = 0, 1, \dots, d-1$ , denote all  $d$  eigenvalues of this restricted operator  $\hat{H}$ ,

$$\hat{H}|\hat{\chi}_k\rangle = \hat{E}_k|\hat{\chi}_k\rangle , \quad k = 0, 1, \dots, d-1 ,$$

ordered according to

$$\hat{E}_0 \leq \hat{E}_1 \leq \dots \leq \hat{E}_{d-1} .$$

Then the  $k$ th eigenvalue  $E_k$  (counting multiplicity) of  $H$  satisfies the inequality

$$\boxed{E_k \leq \hat{E}_k} , \quad k = 0, 1, \dots, d-1 .$$

Assume now that this  $d$ -dimensional subspace  $D_d$  is spanned by some set of  $d$  linearly independent basis vectors  $|\psi_k\rangle$ ,  $k = 0, 1, \dots, d-1$ : Then the set of eigenvalues  $\hat{E}$  may immediately be determined by diagonalizing the  $d \times d$  matrix

$$\left( \langle \psi_i | \hat{H} | \psi_j \rangle \right) , \quad i, j = 0, 1, \dots, d-1 ,$$

i.e., as the  $d$  roots of the characteristic equation

$$\det \left( \langle \psi_i | \hat{H} | \psi_j \rangle - \hat{E} \langle \psi_i | \psi_j \rangle \right) = 0 , \quad i, j = 0, 1, \dots, d-1 .$$

(This becomes clear by expanding any eigenvector of the restricted operator  $\hat{H}$  in terms of the basis vectors  $|\psi_k\rangle$ ,  $k = 0, 1, \dots, d-1$ , of the subspace  $D_d$ .)

### 3.7 Variational Bound for the Ground State [10, 9]

In order to derive, as a first application of the Rayleigh–Ritz variational technique, an upper bound on the ground-state energy eigenvalue  $E_0$ , it is sufficient to focus one’s interest to the case  $k = 0$  (i.e., to consider an only one-dimensional subspace). In this particular case, the min–max principle reduces to

$$E_0 \leq \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} .$$

(This inequality simply states that the ground-state energy  $E_0$  is less than or equal to any expectation value of the Hamiltonian  $H$ .) However, one is certainly entitled to consider simultaneously even sets of one-dimensional trial spaces and to compute optimized upper bounds by the following **prescription** (or “recipe”):

1. Choose a suitable set of trial states  $\{|\psi_\lambda\rangle\}$  (with elements distinguished from each other by some variational parameter  $\lambda$ ). Each of these trial states serves to span a one-dimensional trial space.
2. Calculate the expectation values of the Hamiltonian  $H$  with respect to these trial states  $|\psi_\lambda\rangle$ :

$$E(\lambda) \equiv \frac{\langle \psi_\lambda | H | \psi_\lambda \rangle}{\langle \psi_\lambda | \psi_\lambda \rangle} .$$

3. Determine (from the first derivative of  $E(\lambda)$  with respect to  $\lambda$ ) that value  $\lambda_{\min}$  of the variational parameter  $\lambda$  which minimizes  $E(\lambda)$ .
4. Compute  $E(\lambda_{\min})$  (that is, the minimal expectation value of  $H$  in the Hilbert-space subsector of the chosen trial states  $\{|\psi_\lambda\rangle\}$ ).

When going through these steps, your reward will be an optimized upper bound for the ground state:

$$E_0 \leq E(\lambda_{\min}) .$$

In order to get rid of the troublesome square-root operator in the Hamiltonian  $H$ , one may adopt a trivial (nevertheless fundamental) inequality for the expectation values of a self-adjoint but otherwise arbitrary operator  $\mathcal{O} = \mathcal{O}^\dagger$  and its square, taken with respect to any arbitrary Hilbert-space state  $|\psi\rangle$  in the domain of this operator:

$$\langle \psi | \mathcal{O} | \psi \rangle^2 \leq \langle \psi | \mathcal{O}^2 | \psi \rangle \langle \psi | \psi \rangle$$

and thus

$$\boxed{\frac{|\langle \psi | \mathcal{O} | \psi \rangle|}{\langle \psi | \psi \rangle} \leq \sqrt{\frac{\langle \psi | \mathcal{O}^2 | \psi \rangle}{\langle \psi | \psi \rangle}}}.$$

It should prove to be advantageous to consider the above inequality for the kinetic-energy operator  $T$ :

$$\frac{|\langle \psi | T | \psi \rangle|}{\langle \psi | \psi \rangle} \leq \sqrt{\frac{\langle \psi | T^2 | \psi \rangle}{\langle \psi | \psi \rangle}}.$$

Apply this to the semirelativistic Hamiltonian  $H$ :

$$\begin{aligned} E_0 &\leq \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad (\text{by the min-max principle}) \\ &= \frac{\langle \psi | T + V | \psi \rangle}{\langle \psi | \psi \rangle} \\ &\leq \sqrt{\frac{\langle \psi | T^2 | \psi \rangle}{\langle \psi | \psi \rangle}} + \frac{\langle \psi | V | \psi \rangle}{\langle \psi | \psi \rangle} \quad (\text{by the above inequality}) \\ &\equiv \sqrt{\frac{\langle \psi | \mathbf{p}^2 | \psi \rangle}{\langle \psi | \psi \rangle}} + m^2 + \frac{\langle \psi | V | \psi \rangle}{\langle \psi | \psi \rangle}. \end{aligned}$$

Note, with due satisfaction, that now only the expectation values of  $\mathbf{p}^2$  and of  $V$  have to be evaluated.

For the **Coulomb potential** (2), maybe the first choice for the coordinate-space representation of trial vectors which comes to one's mind are the well-known (normalized) hydrogen-like trial functions

$$\psi_\lambda(\mathbf{x}) = \sqrt{\frac{\lambda^3}{\pi}} \exp(-\lambda r), \quad \lambda > 0.$$

This choice of trial states yields for the expectation values

- of the square of the momentum  $\mathbf{p}$ :

$$\frac{\langle \psi_\lambda | \mathbf{p}^2 | \psi_\lambda \rangle}{\langle \psi_\lambda | \psi_\lambda \rangle} = \lambda^2,$$

- of the inverse of the radial coordinate  $r$ :

$$\frac{\langle \psi_\lambda | r^{-1} | \psi_\lambda \rangle}{\langle \psi_\lambda | \psi_\lambda \rangle} = \lambda.$$

Insertion of these expectation values into the above boundary expression results in the one-parameter set of upper bounds

$$E_0 \leq \sqrt{\lambda^2 + m^2} - \alpha \lambda \quad \text{for all } \lambda > 0,$$

with the absolute minimum

$$\boxed{E_0 \leq m \sqrt{1 - \alpha^2}};$$

this is identical to the previously found generalized operator bound for  $n = 1$ . For  $\alpha \neq 0$  this bound is lower and thus better than the Schrödinger bound on the ground-state energy (which is characterized by the quantum numbers  $n_r = \ell = 0$  and thus  $n = 1$ ):

$$E_{S,0} = m \left( 1 - \frac{\alpha^2}{2} \right).$$

One may conclude that the variational technique yields indeed improved upper bounds on the energy levels.

### 3.8 Energy Levels at the Critical Coupling Constant [11]

For the **Coulomb potential** (2), it might be of interest to derive upper bounds on the energy levels at the critical coupling constant  $\alpha_c$ , particularly, to improve the upper bound on the ground-state energy. A still rather simple-minded but very useful choice for the basis vectors  $|\psi_k\rangle$  (labelled by some positive integer  $k$ , i.e.,  $k = 0, 1, 2, \dots$ ) of the  $d$ -dimensional trial space  $D_d$  is given

- in configuration-space representation by

$$\psi_k(r) = \sqrt{\frac{(2m)^{2k+2\beta+1}}{4\pi\Gamma(2k+2\beta+1)}} r^{k+\beta-1} \exp(-mr), \quad r \equiv |\mathbf{x}|, \quad \beta \geq 0, \quad m > 0,$$

- in momentum-space representation by

$$\tilde{\psi}_k(p) = \sqrt{\frac{(2m)^{2k+2\beta+1}}{2\pi^2\Gamma(2k+2\beta+1)}} \Gamma(k+\beta+1) \frac{\sin\left[(k+\beta+1)\arctan\frac{p}{m}\right]}{p(p^2+m^2)^{(k+\beta+1)/2}}, \quad p \equiv |\mathbf{p}|, \quad \beta \geq 0.$$

Here, the parameter  $\beta$  allows, for a given value of the coupling constant  $\alpha$ , of the total cancellation of the divergent contributions to the expectation values of,

- on the one hand, the kinetic-energy operator  $T$  for large momenta  $p$  and,
- on the other hand, the Coulomb interaction-potential operator  $V_C(r)$  at small distances  $r$ :

$$\beta = \beta(\alpha).$$

The parameter  $\beta$  is implicitly determined as a function of the coupling constant  $\alpha$ , for instance, by the relation<sup>4</sup> [5, 12]

$$\alpha = \beta \cot\left(\frac{\pi}{2}\beta\right) \quad \text{for the ground state}.$$

Hence, the critical coupling constant,  $\alpha_c$ , is approached in the limit of vanishing  $\beta$ , that is, for  $\beta \rightarrow 0$ . For the present choice of trial states, the above-mentioned singularities arise only in matrix elements taken with respect to the ground state  $|\psi_0\rangle$ , i.e., in the matrix elements  $\langle\psi_0|T|\psi_0\rangle$  and  $\langle\psi_0|V_C(r)|\psi_0\rangle$ . For arbitrary parameter value  $\beta$ , the above choice of basis vectors  $|\psi_k\rangle$  implies for the matrix elements

- of the kinetic-energy operator  $T$

$$\begin{aligned} \langle\psi_i|T|\psi_j\rangle &= \frac{2^{i+j+2\beta+1}m}{\pi} \frac{\Gamma(i+\beta+1)\Gamma(j+\beta+1)}{\sqrt{\Gamma(2i+2\beta+1)\Gamma(2j+2\beta+1)}} \\ &\times \int_0^\infty dy \frac{\cos[(i-j)\arctan y] - \cos[(i+j+2\beta+2)\arctan y]}{(1+y^2)^{(i+j+2\beta+1)/2}}, \end{aligned}$$

which has to be evaluated with the help of the expansion

$$\cos(N \arctan y) = \frac{1}{(1+y^2)^{N/2}} \sum_{n=0}^N \binom{N}{n} \cos\left(\frac{n\pi}{2}\right) y^n \quad \text{for } N = 0, 1, 2, \dots;$$

- of the Coulomb interaction-potential operator  $V = V_C(r)$

$$\langle\psi_i|V|\psi_j\rangle = -\frac{2m\alpha\Gamma(i+j+2\beta)}{\sqrt{\Gamma(2i+2\beta+1)\Gamma(2j+2\beta+1)}};$$

- and for the projections of the basis states  $|\psi_k\rangle$  onto each other

$$\langle\psi_i|\psi_j\rangle = \frac{\Gamma(i+j+2\beta+1)}{\sqrt{\Gamma(2i+2\beta+1)\Gamma(2j+2\beta+1)}}.$$

---

<sup>4</sup> Choosing equidistant values for the parameter  $\beta$ , this relation then yields the curious values of the Coulomb coupling constant  $\alpha$  adopted in Tables 1, 2, and 3.

For notational simplicity, define a dimensionless energy eigenvalue  $\varepsilon$  by extracting overall factors:

$$\hat{E} =: \frac{2}{\pi} m \varepsilon .$$

The resulting characteristic equation for the case of relevance here, viz.,  $\beta = 0$ , is typically of the form

$$\det \begin{pmatrix} 4 \ln 2 - 2 - \varepsilon & \frac{\sqrt{2}}{3} - \frac{\varepsilon}{\sqrt{2}} & \cdots \\ \frac{\sqrt{2}}{3} - \frac{\varepsilon}{\sqrt{2}} & \frac{17}{15} - \varepsilon & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} = 0 .$$

The roots of the characteristic equation (which may be calculated algebraically up to  $d = 4$ ) then read,

- for  $d = 1$ ,

$$\varepsilon = 2 (2 \ln 2 - 1) ,$$

which entails, as upper bound for the ground state,

$$\frac{\hat{E}_0}{m} = 0.4918 \dots ;$$

- for  $d = 2$ ,

$$\varepsilon = \frac{1}{15} \left( 60 \ln 2 - 23 \pm \sqrt{(60 \ln 2)^2 - 4800 \ln 2 + 1649} \right) ,$$

which entails, as upper bound for the ground state,

$$\frac{\hat{E}_0}{m} = 0.484288 \dots ;$$

- while, for  $d = 4$ , a lengthy expression for the roots implies, as upper bound for the ground state,

$$\boxed{\frac{\hat{E}_0}{m} = 0.4842564 \dots} .$$

Interestingly, already for  $d = 2$  our (analytical) bound lies well within the numerically obtained range

$$0.4825 \leq \frac{E_0}{m} \leq 0.4842910 \quad \text{for } \alpha = \alpha_c .$$

### 3.9 Generalized Laguerre Basis

Quite generally, upper bounds on eigenvalues may be improved by (suitably) modifying the trial space  $D_d$ , by enlarging it to higher dimensions  $d$  or by spanning it by a more sophisticated set of basis states. A—rather popular—choice of trial functions is based on the generalized Laguerre polynomials  $L_k^{(\gamma)}(x)$  (for the parameter  $\gamma$ ): these are orthogonal polynomials

- defined by the power series

$$L_k^{(\gamma)}(x) = \sum_{t=0}^k (-1)^t \binom{k+\gamma}{k-t} \frac{x^t}{t!}$$

- and normalized, with the weight function  $x^\gamma \exp(-x)$ , according to

$$\int_0^\infty dx x^\gamma \exp(-x) L_k^{(\gamma)}(x) L_{k'}^{(\gamma)}(x) = \frac{\Gamma(\gamma + k + 1)}{k!} \delta_{kk'} .$$

In order to construct trial vectors  $|\psi\rangle$  of the subspace  $D_d$ , corresponding to states with orbital angular momentum  $\ell$  and its projection  $m$ , introduce two variational parameters, namely:

- $\mu$  (with dimension of mass), and
- $\beta$  (dimensionless).

The chosen set of “Laguerre” trial states  $|\psi_k\rangle$  is then defined by the configuration-space representation

$$\psi_{k,\ell m}(\mathbf{x}) = \sqrt{\frac{(2\mu)^{2\ell+2\beta+1} k!}{\Gamma(2\ell+2\beta+k+1)}} r^{\ell+\beta-1} \exp(-\mu r) L_k^{(2\ell+2\beta)}(2\mu r) \mathcal{Y}_{\ell m}(\Omega_{\mathbf{x}}) ,$$

with the spherical harmonics  $\mathcal{Y}_{\ell m}(\Omega)$  for angular momentum  $\ell$  and its projection  $m$ , depending on the solid angle  $\Omega$  and orthonormalized according to

$$\int d\Omega \mathcal{Y}_{\ell m}^*(\Omega) \mathcal{Y}_{\ell' m'}(\Omega) = \delta_{\ell\ell'} \delta_{mm'} .$$

The requirement of normalizability of the (Hilbert-space) trial states  $|\psi_k\rangle$  imposes on the parameters  $\mu$  and  $\beta$  the constraints

$$\mu > 0 , \quad \beta > -\frac{1}{2} .$$

In this case, the configuration-space trial function  $\psi_{k,\ell m}(\mathbf{x})$  satisfies the orthonormalization condition

$$\int d^3x \psi_{k,\ell m}^*(\mathbf{x}) \psi_{k',\ell' m'}(\mathbf{x}) = \delta_{kk'} \delta_{\ell\ell'} \delta_{mm'} .$$

The momentum-space representation of these trial states  $|\psi_k\rangle$  (obtained by Fourier transformation) is

$$\begin{aligned} \tilde{\psi}_{k,\ell m}(\mathbf{p}) &= \sqrt{\frac{(2\mu)^{2\ell+2\beta+1} k!}{\Gamma(2\ell+2\beta+k+1)}} \frac{(-i)^\ell |\mathbf{p}|^\ell}{2^{\ell+1/2} \Gamma(\ell + \frac{3}{2})} \sum_{t=0}^k \frac{(-1)^t}{t!} \binom{k+2\ell+2\beta}{k-t} \\ &\times \frac{\Gamma(2\ell+\beta+t+2) (2\mu)^t}{(\mathbf{p}^2 + \mu^2)^{(2\ell+\beta+t+2)/2}} F\left(\frac{2\ell+\beta+t+2}{2}, -\frac{\beta+t}{2}; \ell + \frac{3}{2}; \frac{\mathbf{p}^2}{\mathbf{p}^2 + \mu^2}\right) \mathcal{Y}_{\ell m}(\Omega_{\mathbf{p}}) , \end{aligned}$$

with the hypergeometric series  $F$ , defined by

$$F(u, v; w; z) = \frac{\Gamma(w)}{\Gamma(u) \Gamma(v)} \sum_{n=0}^{\infty} \frac{\Gamma(u+n) \Gamma(v+n)}{\Gamma(w+n)} \frac{z^n}{n!} .$$

Then trivially, the momentum-space trial function  $\tilde{\psi}_{k,\ell m}(\mathbf{p})$  satisfies the orthonormalization condition

$$\int d^3p \tilde{\psi}_{k,\ell m}^*(\mathbf{p}) \tilde{\psi}_{k',\ell' m'}(\mathbf{p}) = \delta_{kk'} \delta_{\ell\ell'} \delta_{mm'} .$$

### 3.10 Power-Law Potentials [13]

In order to be fairly general, consider an interaction potential of power-law form:

$$V(r) = \sum_n a_n r^{b_n} , \quad r \equiv |\mathbf{x}| ,$$

where the sets of (otherwise arbitrary) real constants  $a_n$  and  $b_n$  are only constrained by the necessary boundedness from below of the Hamiltonian:

$$b_n \geq -1 \quad \text{if} \quad a_n < 0 .$$

The matrix elements of this power-law potential  $V(|\mathbf{x}|)$  are easily worked out:

$$\begin{aligned} \langle \psi_i | V | \psi_j \rangle &= \sqrt{\frac{i! j!}{\Gamma(2\ell+2\beta+i+1) \Gamma(2\ell+2\beta+j+1)}} \sum_n \frac{a_n}{(2\mu)^{b_n}} \sum_{t=0}^i \sum_{s=0}^j \frac{(-1)^{t+s}}{t! s!} \\ &\times \binom{i+2\ell+2\beta}{i-t} \binom{j+2\ell+2\beta}{j-s} \Gamma(2\ell+2\beta+b_n+t+s+1) . \end{aligned}$$

From this expression, the potential matrix  $V \equiv (\langle \psi_i | V | \psi_j \rangle)$  may easily be written down explicitly: if

- considering, for instance, only radial excitations ( $\ell = 0$ ) and
- choosing for the variational parameter  $\beta$  the value  $\beta = 1$ ,

one finds

$$V = \frac{1}{6} \sum_n \frac{a_n}{(2\mu)^{b_n}} \Gamma(3+b_n) \begin{pmatrix} 3 & -\sqrt{3} b_n & \cdots \\ -\sqrt{3} b_n & 3+b_n+b_n^2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} .$$

### 3.11 Analytically Evaluable Special Cases [13]

Compared with the above calculation, an evaluation of the kinetic-energy matrix elements  $\langle \psi_i | T | \psi_j \rangle$  is certainly more delicate. However, there are several situations which allow for an analytical treatment.

#### 3.11.1 Orbital Excitations

Restricting to the case  $i = j = 0$  but allowing for arbitrary values of the orbital angular momentum  $\ell$  means to consider pure orbital excitations. Merely for definiteness, fix, for the moment, the variational parameter  $\beta$  to the value  $\beta = 1$ . In this case, the matrix elements of the power-law potential operator simplify to

$$\langle \psi_0 | V | \psi_0 \rangle = \frac{1}{\Gamma(2\ell + 3)} \sum_n \frac{a_n}{(2\mu)^{b_n}} \Gamma(2\ell + b_n + 3) ,$$

while a rather straightforward calculation yields for the matrix elements of the kinetic-energy operator

$$\langle \psi_0 | T | \psi_0 \rangle = \frac{4^{\ell+2} [\Gamma(\ell + 2)]^2}{\sqrt{\pi} \Gamma(2\ell + \frac{7}{2})} \mu F\left(-\frac{1}{2}, \ell + 2; 2\ell + \frac{7}{2}; 1 - \frac{m^2}{\mu^2}\right) .$$

Aiming at analytical results, one should clearly try to get rid of the hypergeometric series  $F$ . There are several possibilities to do so:

- In the ultrarelativistic limit (realized for vanishing particle mass,  $m = 0$ ), by use of the relation

$$F(u, v; w; 1) = \frac{\Gamma(w) \Gamma(w - u - v)}{\Gamma(w - u) \Gamma(w - v)} \quad \text{for } w \neq 0, -1, -2, \dots, \Re(w - u - v) > 0 ,$$

the above kinetic-energy matrix element simplifies to

$$\langle \psi_0 | T | \psi_0 \rangle = \frac{2 [\Gamma(\ell + 2)]^2}{\Gamma(\ell + \frac{3}{2}) \Gamma(\ell + \frac{5}{2})} \mu .$$

For instance, for the **linear potential**

$$V(r) = a r , \quad a > 0 ,$$

minimizing the expectation value  $\langle \psi_0 | H | \psi_0 \rangle$  with respect to the variational parameter  $\mu$  leads to the minimal upper bound

$$\boxed{\min_{\mu > 0} \langle \psi_0 | H | \psi_0 \rangle = 2 \Gamma(\ell + 2) \sqrt{\frac{(2\ell + 3) a}{\Gamma(\ell + \frac{3}{2}) \Gamma(\ell + \frac{5}{2})}} = 2 \sqrt{2a} \frac{\Gamma(\ell + 2)}{\Gamma(\ell + \frac{3}{2})} .}$$

In the limit of large orbital angular momenta ( $\ell \rightarrow \infty$ ), this optimized upper bound reduces to

$$\lim_{\ell \rightarrow \infty} \left( \min_{\mu > 0} \langle \psi_0 | H | \psi_0 \rangle \right)^2 = 8 a \left( \ell + \frac{5}{4} \right) .$$

Consequently, it describes linear Regge trajectories:<sup>5</sup>

$$[E(\ell)]^2 \propto \ell ,$$

which is in striking accordance with all other findings based on different considerations [14, 15].

- Another possibility—which will not be followed any longer—is to fix the variational parameter  $\mu$  to the value  $\mu = m$  (which reduces the last argument of the hypergeometric series  $F$  to 0) and to take advantage of the relation

$$F(u, v; w; 0) = 1 ,$$

in order to obtain the kinetic-energy matrix element

$$\langle \psi_0 | T | \psi_0 \rangle = \frac{4^{\ell+2} [\Gamma(\ell + 2)]^2}{\sqrt{\pi} \Gamma(2\ell + \frac{7}{2})} m .$$

---

<sup>5</sup> The square of the exact optimized bound is already almost perfectly linear. Its deviation from the asymptotic linearity is monotonously decreasing for increasing angular momentum  $\ell$ . The maximum relative deviation (occurring clearly at the point  $\ell = 0$ ) is  $1 - 5\pi/16 = 1.8\%$ .



### 3.11.2 Radial Excitations

Focusing one's interest exclusively to states with vanishing orbital angular momentum  $\ell$  ( $\ell = 0$ ) means to consider only radial excitations. The matrix elements of the kinetic-energy operator then typically take the form

$$\begin{aligned} \langle \psi_i | T | \psi_j \rangle &= \sqrt{\frac{i! j!}{\Gamma(2\beta + i + 1) \Gamma(2\beta + j + 1)}} \frac{4^{\beta+1}}{2\pi} \mu \sum_{t=0}^i \sum_{s=0}^j \frac{(-2)^{t+s}}{t! s!} \\ &\times \binom{i+2\beta}{i-t} \binom{j+2\beta}{j-s} \Gamma(\beta + t + 1) \Gamma(\beta + s + 1) I_{ts} , \end{aligned}$$

with some integral  $I_{ts}$  which under certain circumstances may be calculated analytically. For instance, for  $\mu = m$ , and for  $2\beta$  integer and thus (remembering the above normalizability constraint  $2\beta > -1$ ) non-negative, i.e.,  $2\beta = 0, 1, 2, \dots$ , one easily finds

$$\begin{aligned} I_{ts} &= \frac{1}{2} \left[ \Gamma \left( \frac{2\beta + t + s + |t-s| + 1}{2} \right) \right]^{-1} \sum_{n=0}^{|t-s|} \binom{|t-s|}{n} \\ &\times \Gamma \left( \frac{n+1}{2} \right) \Gamma \left( \frac{2\beta + t + s + |t-s| - n}{2} \right) \cos \left( \frac{n\pi}{2} \right) \\ &- \frac{1}{2} \left[ \Gamma \left( 2\beta + t + s + \frac{3}{2} \right) \right]^{-1} \sum_{n=0}^{2\beta+t+s+2} \binom{2\beta+t+s+2}{n} \\ &\times \Gamma \left( \frac{n+1}{2} \right) \Gamma \left( 2\beta + t + s + 1 - \frac{n}{2} \right) \cos \left( \frac{n\pi}{2} \right) . \end{aligned}$$

With this result, the kinetic-energy matrix  $T \equiv (\langle \psi_i | T | \psi_j \rangle)$  reads, for variational parameter  $\beta$  fixed to  $\beta = 1$ , explicitly:

$$T = \frac{64}{15\pi} m \begin{pmatrix} 1 & \frac{\sqrt{3}}{7} & \dots \\ \frac{\sqrt{3}}{7} & \frac{11}{9} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} .$$

In this way, analytic expressions for the matrix elements  $\langle \psi_i | H | \psi_j \rangle$  of the semirelativistic Hamiltonian  $H$  with power-law potential may be found.

- Up to a trial-space dimension  $d = 4$  these matrix elements are, at least in principle, algebraically accessible.
- For larger trial-space dimension, i.e.,  $d > 4$ , the energy matrix  $(\langle \psi_i | H | \psi_j \rangle)$  must be diagonalized numerically, without, however, the necessity to invoke (time-consuming) integration procedures.

In order to estimate the quality of all the upper bounds derived, consider, for the following reason, the **harmonic-oscillator potential**

$$V(r) = \omega r^2 , \quad \omega > 0 .$$

In momentum space the operator  $r^2$  is represented by the Laplacian with respect to the momentum  $\mathbf{p}$ ,

$$r^2 \longrightarrow \Delta_{\mathbf{p}} ,$$

while the kinetic energy, nonlocal in configuration space, is represented by a multiplication operator. Consequently, the semirelativistic Hamiltonian  $H$  in momentum-space representation is equivalent to a nonrelativistic Hamiltonian with some effective (square-root) interaction potential. The equation of motion resulting in this way is then solvable with one of the numerous numerical procedures designed for the treatment of the nonrelativistic Schrödinger equation. For the **comparison** (Table 4) of these Laguerre bounds with results of a numerical solution of the (“momentum-space,” in the above sense) Schrödinger equation, we employ some standard set of parameter values [16]:  $m = 2 \text{ GeV}$ ,  $\omega = 2 \text{ GeV}^3$  (as well as the choice  $\mu = m$ ,  $\beta = 1$ ); we observe a rapid convergence of our upper bounds towards the

Table 4: Upper bounds (in units of GeV) on energy levels (labelled in usual spectroscopic notation) for a  $d \times d$  energy matrix. (Analytically obtained results in italics.)

State	$1 \times 1$	$2 \times 2$	$25 \times 25$	Schrödinger
1S	<i>4.2162</i>	<i>3.9276</i>	3.8249	3.8249
2S	—	<i>8.1085</i>	5.7911	5.7911
3S	—	—	7.4829	7.4823
4S	—	—	9.0215	9.0075

## 4 SUMMARY

The min–max principle and related simple theorems allow to derive rigorous statements on the energy levels predicted by a bound-state wave equation like the spinless Salpeter equation. In principle, these methods should work for all physical situations which may be formulated as an eigenvalue problem. If one is not satisfied with the outcome of this procedure, or if one is interested in the corresponding wave functions, one has to actually solve the equation of motion by some numerical approximation method. The most efficient among these is perhaps the “semianalytical matrix method” proposed in Ref. [17]. Nevertheless, there still remain questions of the significance [16] of too naive relativistic improvements of some nonrelativistic potential models for the description of hadrons as bound states of quarks [18].

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